We Claim:

1. A composition comprising a polypeptide in crystalline form, wherein the polypeptide is a TNF-α-converting enzyme (TACE) polypeptide.

2. A composition according to claim 1, wherein the TACE polypeptide comprises the TACE catalytic domain (TCD).

3. A composition according to claim 1, wherein the TACE polypeptide is the expression product of a polynucleotide encoding the pro and catalytic domains of TACE.

4. A composition according to claim 1, wherein the TACE polypeptide is the expression product of a polynucleotide encoding the amino acid residues 1-477 of TACE.

5. A composition according to claim 4, wherein the polynucleotide is substituted such that amino acid residue Ser266 is changed to Ala and amino acid residue Asn542 is changed to Gln, and wherein a second polynucleotide encoding the sequence Gly-Ser-$(His)_6$ is fused to the C-terminus.

6. A composition according to claim 1, further comprising a binding partner suitable for co-crystallization with the TACE polypeptide.

7. A composition according to claim 6, wherein the binding partner is a hydroxamate-based binding partner.

8. A composition according to claim 6, wherein the binding partner is N-{D,L-2-(hydroxyaminocarbonyl)methyl-4-methylpentanoyl}-L-3-amino-2-dimethylbutanoyl-L-alanine,2-(amino)ethyl amide.

9. A composition according to claim 1, wherein the crystal has a crystal structure diffracting to 2.0 Å.

10. A composition according to claim 1, wherein the crystal is monoclinic.

11. A composition according to claim 1, wherein the unit cell of the crystal comprises four crystallographically independent TCD molecules.

12. A composition according to claim 11, wherein the TCD molecules are in an asymmetric unit.

13. A composition according to claim 1, wherein the crystal is of monoclinic space group $P2_1$ and the cell has the constants a=61.38 A, b=126.27 A, c=81.27 A, and β=107.41°.

14. A composition according to claim 1, wherein the polypeptide is characterized by the structure coordinates according to Table 1, or a substantial part thereof.

15. A method for crystallizing a TACE polypeptide, comprising:

(A) mixing a solution comprising a TACE polypeptide and a binding partner with a crystallization buffer; and

(B) crystallizing the mixture of step (A) by drop vapor diffusion to form a crystalline precipitate.

16. The method according to claim 15, further comprising:

(C) transferring seeds from the crystalline precipitate formed by the drop vapor diffusion, along with a crystallization promoter, into a mixture of a concentrated solution comprising a TACE polypeptide and binding partner substrate, and a crystallization buffer; and

(D) crystallizing the mixture of step (C) by drop vapor diffusion to form a crystal.

17. The method of claim 15, wherein said crystallization buffer is 0.1M Na Citrate pH 5.4, 20%w/v PEG 4000, and 20% v/v isopropanol.

18. The method of claim 15, wherein the binding partner is N-{D,L-2-(hydroxyaminocarbonyl)methyl-4-methylpentanoyl}-L-3-amino-2-dimethylbutanoyl-L-alanine, 2-(amino)ethyl amide.

19. The method of claim 15, wherein crystallization is at a temperature ranging from 4 to 20 degrees Celsius.

20. The method of claim 15, wherein the solution comprising the TACE polypeptide and the binding partner is at a concentration of about 5 mg/mL to about 12 mg/mL in a buffer.

21. The method of claim 20, wherein the solution is mixed with the crystallization buffer in a 1:1 ratio.

22. A TACE crystal made by co-crystallizing a TACE polypeptide with a co-crystallization substrate.

23. A method of identifying a compound that associates with TACE, comprising (A) designing a compound that associates with a catalytic domain of a TACE polypeptide, using atomic coordinates from a region selected from the group consisting of the S1' region, the S1'S3' pocket and atoms which bind a catalytic zinc, (B) synthesizing said compound, and (C) determining *in vitro* whether said compound associates with said catalytic domain,
wherein said atomic coordinates are selected from Table 1.

24. The method of claim 23, wherein said region comprises the atomic coordinates for the S1' region.

25. The method of claim 23, wherein said region comprises the atomic coordinates for the S1'S3' pocket.

26. The method of claim 23, wherein said region comprises the atomic coordinates for atoms which bind a catalytic zinc.

27. The method of claim 26, wherein said atoms comprise atoms His405, His409 and His415.